FULL ESTIMATED COST 166.94 167.15

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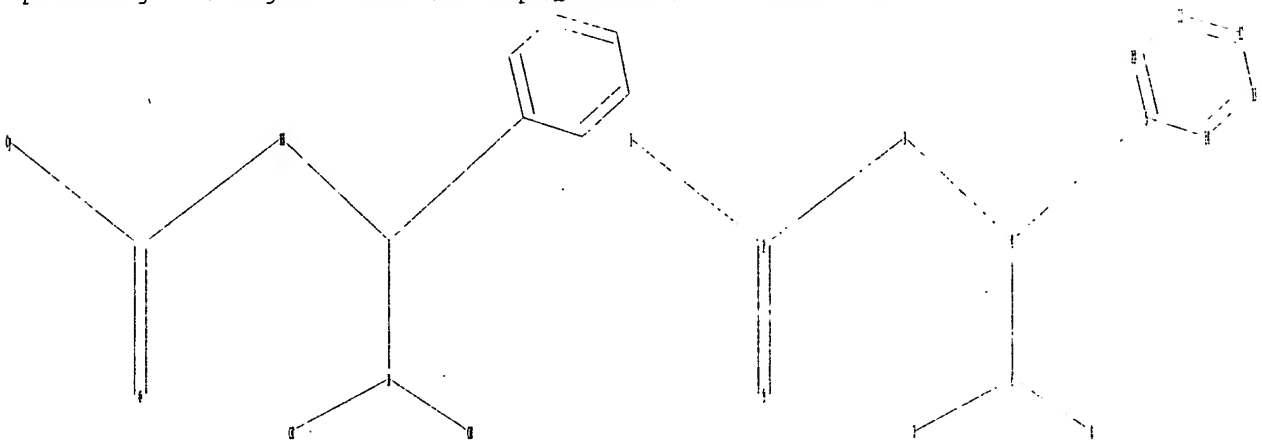
http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10731738s2.str



chain nodes :
1 2 3 4 6 7 8 9
ring nodes :
5 10 11 12 13 14
chain bonds :
1-2 2-3 2-9 3-4 4-5 4-6 6-7 6-8
ring bonds :
5-10 5-14 10-11 11-12 12-13 13-14
exact/norm bonds :
1-2 2-3 2-9 3-4
exact bonds :
4-5 4-6 6-7 6-8
normalized bonds :
5-10 5-14 10-11 11-12 12-13 13-14

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PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

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NEWS 4	APR 04	STN AnaVist $500 visualization usage credit offered
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NEWS 7	MAY 19	Derwent World Patents Index to be reloaded and enhanced
NEWS 8	MAY 30	IPC 8 Rolled-up Core codes added to CA/CAplus and USPATFULL/USPAT2
NEWS 9	MAY 30	The F-Term thesaurus is now available in CA/CAplus
NEWS 10	JUN 02	The first reclassification of IPC codes now complete in INPADOC
NEWS 11	JUN 26	TULSA/TULSA2 reloaded and enhanced with new search and and display fields
NEWS 12	JUN 28	Price changes in full-text patent databases EPFULL and PCTFULL
NEWS 13	JUl 11	CHEMSAFE reloaded and enhanced
NEWS 14	JUl 14	FSTA enhanced with Japanese patents
NEWS 15	JUl 19	Coverage of Research Disclosure reinstated in DWPI

NEWS EXPRESS JUNE 30 CURRENT WINDOWS VERSION IS V8.01b, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 26 JUNE 2006.

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NEWS LOGIN	Welcome Banner and News Items
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FILE 'HOME' ENTERED AT 16:00:35 ON 28 JUL 2006

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

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DICTIONARY FILE UPDATES: 27 JUL 2006 HIGHEST RN 896463-29-9

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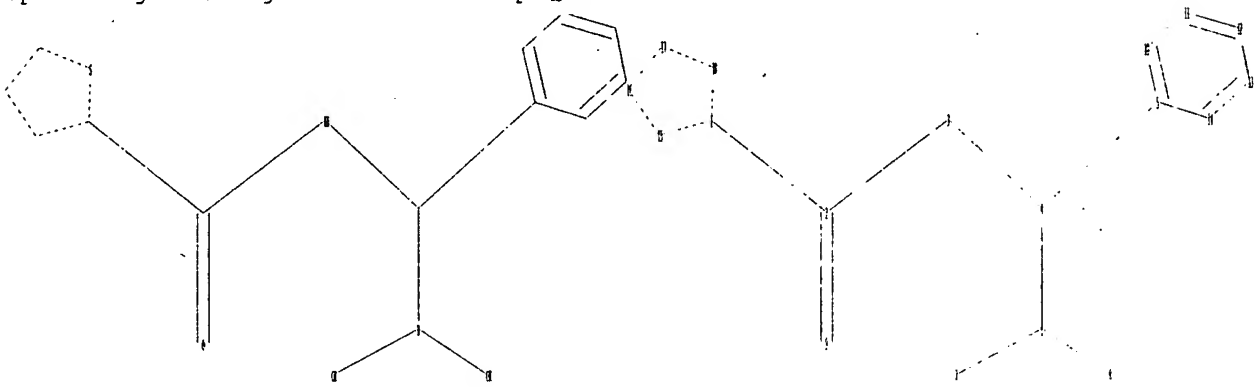
http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10731738s.str

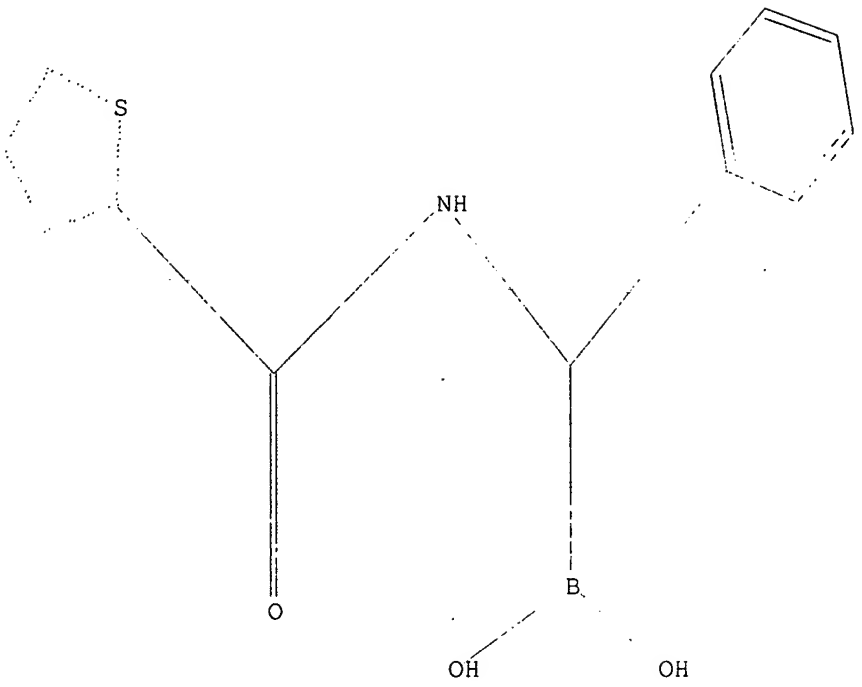


chain nodes :
2 3 4 6 7 8 9
ring nodes :
1 5 10 11 12 13 14 15 16 17 18
chain bonds :
1-2 2-3 2-9 3-4 4-5 4-6 6-7 6-8
ring bonds :
1-15 1-18 5-10 5-14 10-11 11-12 12-13 13-14 15-16 16-17 17-18
exact/norm bonds :
1-15 1-18 2-3 2-9 3-4 15-16 16-17 17-18
exact bonds :
1-2 4-5 4-6 6-7 6-8
normalized bonds :
5-10 5-14 10-11 11-12 12-13 13-14

Match level :
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 16:00:59 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1 TO 80
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 16:01:02 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 19 TO ITERATE

100.0% PROCESSED 19 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

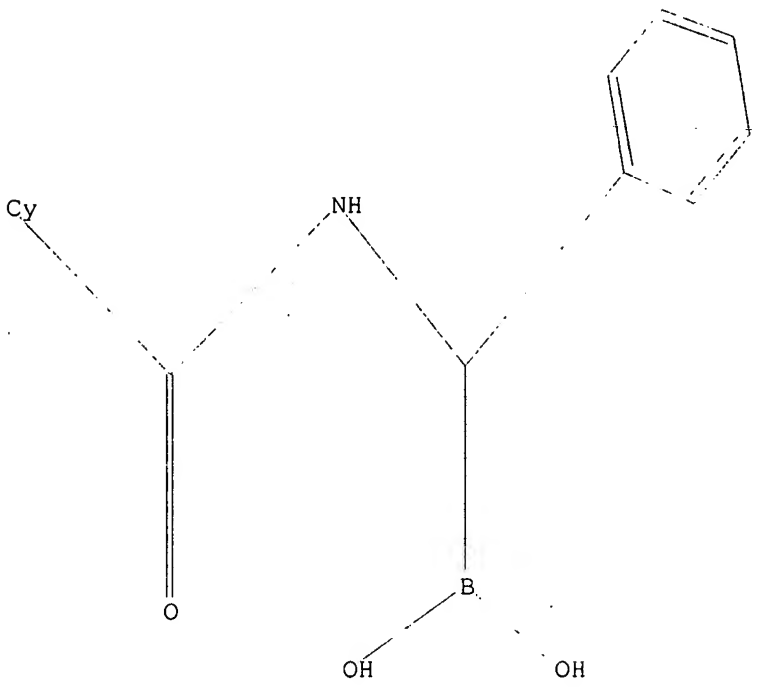
L3 0 SEA SSS FUL L1

=> fil reg
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION

Match level :
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom

L4 STRUCTURE UPLOADED

=> d
L4 HAS NO ANSWERS
L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l4
SAMPLE SEARCH INITIATED 16:02:10 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 23 TO ITERATE

100.0% PROCESSED 23 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 173 TO 747
PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4

=> s l4 full
FULL SEARCH INITIATED 16:02:13 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 607 TO ITERATE

100.0% PROCESSED 607 ITERATIONS 6 ANSWERS
SEARCH TIME: 00.00.01

```
L6             6 SEA SSS FUL L4

=> fil caplus
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     167.38     334.53

FILE 'CAPLUS' ENTERED AT 16:02:16 ON 28 JUL 2006
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FILE LAST UPDATED: 27 Jul 2006  (20060727/ED)

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=> s l6
L7             4 L6

=> d ibib abs hitstr tot
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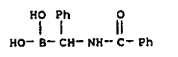
L7 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:980920 CAPLUS
DOCUMENT NUMBER: 143:415326
TITLE: Enantiomeric excess of 1,2-diols by formation of cyclic boronates: an improved method
AUTHOR(S): Morandi, Stefania; Caselli, Emilia; Forni, Arrigo; Bucciarelli, Maria; Torre, Giovanni; Prati, Fabio
CORPORATE SOURCE: Dipartimento di Chimica, Universita di Modena e Reggio Emilia, Modena, 41100, Italy
SOURCE: Tetrahedron: Asymmetry (2005), 16(17), 2918-2926 CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A reliable method for determining the enantiomeric composition of 1,2-diols by the formation of diastereomeric cyclic esters with boronic acid is described. Starting from a previously reported structure of boronic chiral derivatizing agent (CDA), seven structurally related racemic CDAs were synthesized and their discriminating ability towards diols measured. The most promising amongst these was synthesized in its enantiomerically pure form according to Matteson's protocol for the stereoselective homologation of pinanediol boronates; this CDA quant. and rapidly reacts with 1,2-diols in very mild conditions affording a couple of diastereoisomers, whose composition can be determined via 1H NMR anal. In particular, an attractive feature is that the resonance used for the anal. originated from the CDA as a couple of baseline-separated singlets ($\Delta\delta$ up to 0.3 ppm) is useful for integration.

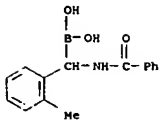
IT 98541-61-8 867182-00-1 867182-01-2 867182-03-4
RL: ARG (Analytical reagent use); PRP (Properties); ANST (Analytical study); USES (Uses)
(determination of enantiomeric excess of 1,2-diols by formation of cyclic boronates)

RN 98541-61-8 CAPLUS
CN Boronic acid, [(benzoylamino)phenylmethyl]- (9CI) (CA INDEX NAME)

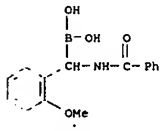


RN 867182-00-1 CAPLUS
CN Boronic acid, [(benzoylamino)(2-methylphenyl)methyl]- (9CI) (CA INDEX NAME)

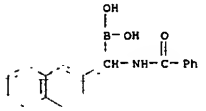
L7 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 867182-01-2 CAPLUS
CN Boronic acid, [(benzoylamino)(2-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



RN 867182-03-4 CAPLUS
CN Boronic acid, [(benzoylamino)-2-naphthalenylmethyl]- (9CI) (CA INDEX NAME)

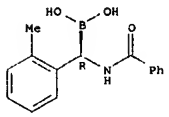


IT 867182-04-5P
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(determination of enantiomeric excess of 1,2-diols by formation of cyclic boronates)

RN 867182-04-5 CAPLUS
CN Boronic acid, [(R)-(benzoylamino)(2-methylphenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

L7 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:478576 CAPLUS
DOCUMENT NUMBER: 139:175717
TITLE: Recognition and resistance in TEM β-lactamase
AUTHOR(S): Wang, Xiaojun; Minasov, George; Blazquez, Jesus; Caselli, Emilia; Prati, Fabio; Shoichet, Brian K.
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, University of California San Francisco, San Francisco, CA, 94143, USA
SOURCE: Biochemistry (2003), 42(28), 8434-8444 CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

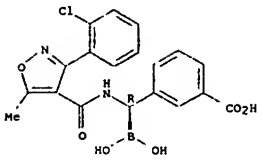
AB Developing antimicrobials that are less likely to engender resistance has become an important design criterion as more and more drugs fall victim to resistance mutations. One hypothesis is that the more closely an inhibitor resembles a substrate, the more difficult it will be to develop resistant mutations that can at once disfavor the inhibitor and still recognize the substrate. To investigate this hypothesis, 10 transition-state analogs, of greater or lesser similarity to substrates, were tested for inhibition of TEM-1 β-lactamase, the most widespread resistance enzyme to penicillin antibiotics. The inhibitors were also tested against four characteristic mutant enzymes: TEM-30, TEM-32, TEM-52, and TEM-64. The inhibitor most similar to the substrate, compound 10, was the most potent inhibitor of the WT enzyme, with a Ki value of 64 nM. Conversely, compound 10 was the most susceptible to the TEM-30 (R244S) mutant, for which inhibition dropped by over 100-fold. The other inhibitors were relatively impervious to the TEM-30 mutant enzyme. To understand recognition and resistance to these transition-state analogs, the structures of four of these inhibitors in complex with TEM-1 were determined by x-ray crystallog. These structures suggest a structural basis for distinguishing inhibitors that mimic the acylation transition state and those that mimic the deacylation transition state; they also suggest how TEM-30 reduces the affinity of compound 10. In cell culture, this inhibitor reversed the resistance of bacteria to ampicillin, reducing min. inhibitory concns. of this penicillin by between 4- and 64-fold, depending on the strain of bacteria. Notwithstanding this activity, the resistance of TEM-30, which is already extant in the clinic, suggests that there can be resistance liabilities with substrate-based design.

IT 497258-68-1
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(transition state analog recognition and inhibition by TEM β-lactamase mutants in relation to antibiotic resistance)

RN 497258-68-1 CAPLUS
CN Benzoic acid, 3-[(R)-boronol[[3-(2-chlorophenyl)-5-methyl-4-isoxazolyl]carbonyl]amino]methyl]- (9CI) (CA INDEX NAME)

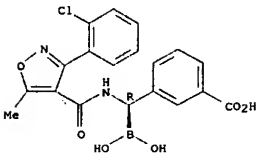
Absolute stereochemistry. Rotation (-).

L7 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:977460 CAPLUS
DOCUMENT NUMBER: 138:165634
TITLE: Nanomolar Inhibitors of AmpC β-Lactamase
AUTHOR(S): Morandi, Federica; Caselli, Emilia; Morandi, Stefania; Focia, Pamela J.; Blazquez, Jesus; Shoichet, Brian K.; Prati, Fabio
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, University of California, San Francisco, CA, 94143, USA
SOURCE: Journal of the American Chemical Society (2003), 125(3), 685-695
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:165634

AB β-Lactamases are the most widespread resistance mechanism to β-lactam antibiotics, such as the penicillins and the cephalosporins. In an effort to combat these enzymes, a combination of stereoselective organic synthesis, enzymol., microbiol., and X-ray crystallog. was used to design and evaluate new carboxyphenyl-glycylboronic acid transition-state analog inhibitors of the class C β-lactamase AmpC. The new compds. improve inhibition by over 2 orders of magnitude compared to analogous glycylboronic acids, with Ki values as low as 1 nM. On the basis of the differential binding of different analogs, the introduced carboxylate alone contributes about 2.1 kcal/mol in affinity. This carboxylate corresponds to the ubiquitous C3(4)' carboxylate of β-lactams, and this energy represents the first thermodn. measurement of the importance of this group in mol. recognition by class C β-lactamases. The structures of AmpC in complex with two of these inhibitors were determined by X-ray crystallog. at 1.72 and 1.83 Å resolution These structures suggest a structural basis for the high affinity of the new compds. and provide templates for further design. The highest affinity inhibitor was 5 orders of magnitude more selective for AmpC than for characteristic serine proteases, such as chymotrypsin. This inhibitor reversed the resistance of clin. pathogens to the third generation cephalosporin ceftazidime; it may serve as a lead compound for drug discovery to combat bacterial resistance to β-lactam antibiotics.

IT 497258-68-1P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(carboxyphenyl-glycylboronic acid transition-state analog inhibitors can inhibit AmpC β-lactamase)

RN 497258-68-1 CAPLUS
CN Benzoic acid, 3-[(R)-borono[[3-(2-chlorophenyl)-5-methyl-4-isoxazolyl]carbonyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L7 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:596378 CAPLUS
DOCUMENT NUMBER: 103:196378
TITLE: Acylamido boronic acids and difluoroborane analogs of amino acids: potent inhibitors of chymotrypsin and elastase
AUTHOR(S): Kinder, David H.; Katzenellenbogen, John A.
CORPORATE SOURCE: Sch. Chem. Sci., Univ. Illinois, Urbana, IL, 61801, USA
SOURCE: Journal of Medicinal Chemistry (1985), 28(12), 1917-25
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 103:196378

AB 1-Acylaminoboronic acid analogs R1CONHCHRBR22 [I; R = CH2Ph, Ph, Me, CHMe2, CHMeEt; R1CO = Ac, Bz, PhCH2O2C-X (X = Ala, Gly); R2 = OH] were prepared as potential transition-state inhibitors of the serine proteases α-chymotrypsin and elastase by a boronate homologation reaction. The corresponding difluoroboranes I (R2 = F), produced from the boronic acids by treatment with HF, were more easily purified than the boronic acids. Since the difluoroboranes readily hydrolyze in water, they are convenient precursors for the boronic acids. The phenylalanine and phenylglycine analogs I (R = CH2Ph, Ph) were good competitive inhibitors of α-chymotrypsin, and the alanine, valine, and isoleucine analogs I (R = Me, CHMe2, CHMeEt) were good inhibitors of elastase. On the basis of their high affinity and the tendency of boronic acids to form borate complexes, these acylamino boronic acids may behave as transition-state inhibitors.

IT 98541-61-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(fluorination of)

RN 98541-61-8 CAPLUS
CN Boronic acid, [(benzoylamino)phenylmethyl]- (9CI) (CA INDEX NAME)

=> fil reg
COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION
FULL ESTIMATED COST | 21.36 | 355.89

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION
CA SUBSCRIBER PRICE | -3.00 | -3.00

FILE 'REGISTRY' ENTERED AT 16:03:30 ON 28 JUL 2006
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provided by InfoChem.

STRUCTURE FILE UPDATES: 27 JUL 2006 HIGHEST RN 896463-29-9
DICTIONARY FILE UPDATES: 27 JUL 2006 HIGHEST RN 896463-29-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

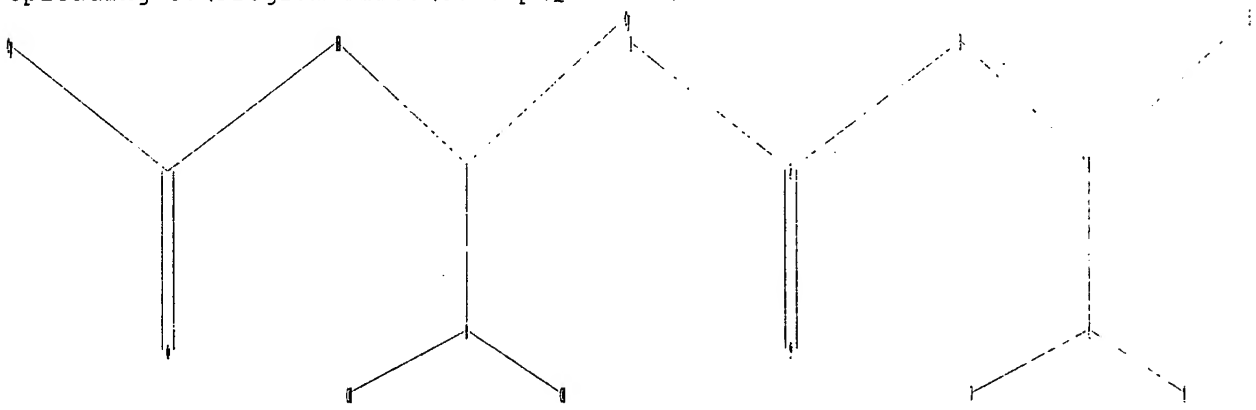
TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10731738s3.str



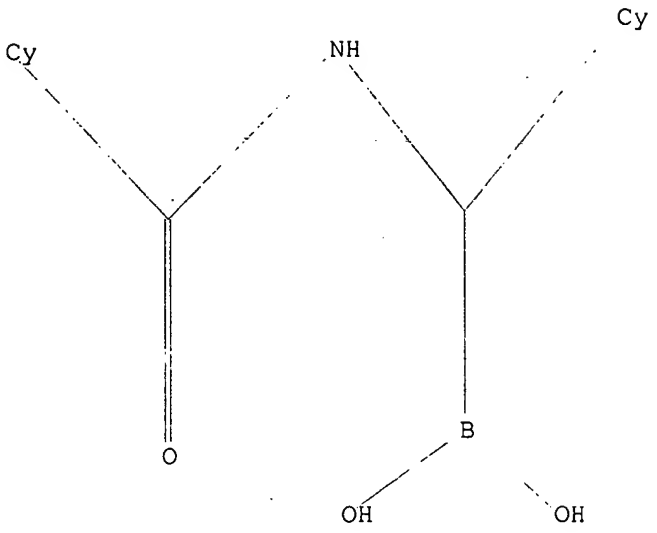
chain nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
1-2 2-3 2-9 3-4 4-5 4-6 6-7 6-8
exact/norm bonds :
1-2 2-3 2-9 3-4 4-5
exact bonds :

4-6 6-7 6-8

Match level :
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS

L8 STRUCTURE UPLOADED

=> d
L8 HAS NO ANSWERS
L8 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l8
SAMPLE SEARCH INITIATED 16:03:41 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 366 TO ITERATE

100.0% PROCESSED 366 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS: 6173 TO 8467
PROJECTED ANSWERS: 0 TO 0

L9 0 SEA SSS SAM L8

=> s l8 full
FULL SEARCH INITIATED 16:03:46 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 6786 TO ITERATE

100.0% PROCESSED 6786 ITERATIONS 6 ANSWERS
SEARCH TIME: 00.00.01

L10 6 SEA SSS FUL L8

=> fil caplus
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	166.94	522.83

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-3.00

FILE 'CAPLUS' ENTERED AT 16:03:49 ON 28 JUL 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 28 Jul 2006 VOL 145 ISS 6
FILE LAST UPDATED: 27 Jul 2006 (20060727/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l10
L11 4 L10

=> log y
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.46	523.29

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-3.00

STN INTERNATIONAL LOGOFF AT 16:03:55 ON 28 JUL 2006